

# Ensemble Inequivalence: A Formal Approach

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## Abstract

Ensemble inequivalence has been observed in several systems. In particular it has been recently shown that negative specific heat can arise in the microcanonical ensemble in the thermodynamic limit for systems with long-range interactions. We display a connection between such behaviour and a mean-field like structure of the partition function. Since short-range models cannot display this kind of behaviour, this strongly suggests that such systems are necessarily non-mean field in the sense indicated here. We further show that a broad class of systems with non-integrable interactions are indeed of mean-field type in the sense specified, so that they are expected to display ensemble inequivalence as well as the peculiar behaviour described above in the microcanonical ensemble.

*Key words:* Long-range interactions, Ensemble inequivalence

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## 1 Introduction

Particle or spin systems for which the pairwise interaction potential decays at large distances with a power smaller than space dimension are called *long-range* or *non-integrable*. It has been suggested [1,2] that at first order phase transitions such systems should display ensemble inequivalence also in the thermodynamic limit. A few examples where this is explicitly shown have been published [1,3–5]. The specific heat, which is always positive in the canonical ensemble, may become negative in the microcanonical, even if the interaction is not singular at short distances like for gravity [6]. Moreover, temperature jumps at critical energies may be present. In this paper we present a formal approach within which all these features can be put into context. The approach

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is based on the assumption, which we justify afterwards, that a sort of Landau free energy can be always introduced for long-range systems.

## 2 Mean-field and Ensemble Inequivalence

In this section, we show the main result of this paper. We say that a system is of *mean-field type* if it satisfies the following condition:

$$Z_c(\beta) = \int_{-\infty}^{\infty} \exp[-N\Psi(\beta, m)] dm, \quad (1)$$

where  $Z_c(\beta)$  is the canonical partition function and  $\Psi(\beta, m)$  is an analytic function of  $\beta$  and  $m$ . Note that we require this for finite values of  $N$ , but that we additionally require the function  $\Psi(\beta, m)$  to be independent of  $N$ . Infinite range models always have this property, as follows from their solution.

From this we can derive that ensemble inequivalence will in general occur. Indeed, from (1) one obtains the following expression for the microcanonical partition function:

$$Z_m(\epsilon) = \int_{-\infty}^{\infty} dm \int_{-i\infty}^{i\infty} \frac{d\lambda}{2\pi i} \exp[N(\lambda\epsilon - \Psi(\lambda, m))]. \quad (2)$$

One can now perform a saddle point integral to estimate the value of the  $\lambda$  integral for large values of  $N$ . We argue that the dominant saddle point must lie on the real axis: If it were otherwise, we would have two complex conjugate dominant saddle points, and hence an oscillatory behaviour of the partition function, contradicting positivity of  $Z_c(\beta)$ . We may therefore limit ourselves to the consideration of real saddle points. Since the integration path is perpendicular to the real axis, the real minima of the argument of the exponential will correspond to allowed saddles, since these will correspond to local maxima when traversed along the imaginary axis. One is thus led to the following expression for the microcanonical entropy per particle:

$$S_m(\epsilon) = \max_m \min_{\lambda} [\lambda\epsilon - \Psi(\lambda, m)]. \quad (3)$$

This result can now be compared with the standard result for the canonical ensemble:

$$S_c(\epsilon) = \min_{\lambda} \max_m [\lambda\epsilon - \Psi(\lambda, m)]. \quad (4)$$

From these formulas, a few consequences are immediate:

- (1) The two forms of the entropy need not be equal. Indeed, if we could prove that  $\Psi(\lambda, m)$  has a unique extremum under certain conditions, we could argue for equality. However, we know that this is not generally the case: Whenever a phase transition occurs, the function  $\Psi(\lambda, m)$  may have multiple extrema at least as a function of  $m$ , thus precluding any simple statements about the identity of the two entropies.
- (2) Let us consider the behaviour of the function  $\Psi$  at its equilibrium points in the two ensembles. For the canonical problem we find the usual stability conditions for the thermodynamic potential  $\Psi$ . However, if one goes through the same computation for the microcanonical ensemble, one finds that concavity in  $\lambda$  and indefiniteness of the Hessian are sufficient for stability. Note in particular how this allows the second derivative of  $\Psi$  with respect to  $m$  to take either sign.
- (3) The microcanonical entropy is a maximum over concave functions, which need not be concave. Specifically, an explicit evaluation of the second derivative of  $S_m(\epsilon)$  yields

$$\frac{d^2 S_m}{d\epsilon^2} = \frac{\partial^2 \Psi}{\partial \lambda^2} - \frac{(\partial^2 \Psi / \partial m \partial \lambda)^2}{\partial^2 \Psi / \partial m^2}. \quad (5)$$

Again, since  $\partial^2 \Psi / \partial m^2$  can take both signs, one sees that the specific heat can do so as well. In fact, one finds that the sign of  $d^2 S_m / d\epsilon^2$  is the opposite of that of  $\partial^2 \Psi / \partial m^2$ . The specific heat is thus negative exactly when the value of  $m$  corresponding to microcanonical equilibrium is unstable from the point of view of the canonical ensemble.

In the canonical case, it can also be shown using standard properties of the Legendre transform that the canonical entropy (4) cannot have a discontinuous derivative. Again, it can be seen both from a general point of view and via explicit examples, that this reasoning does not hold for the microcanonical entropy (3). This means that temperature can be a discontinuous function of energy.

- (4) Finally, we note that, since the equivalence between ensembles is rigorously proved for interactions which are of sufficiently short-range, our arguments strongly suggest that for these systems such functions as  $\Psi$  do not have the required analyticity properties. The argument is not fully rigorous, but it is certainly very suggestive.

### 3 Models with Long-range Interactions

In this Section, we show that a large class of models having non-integrable interactions, actually satisfy our criterion (1). For definiteness' sake we restrict

ourselves to spin models on a lattice. Consider the following Hamiltonian

$$H[s(\vec{i})] = L^{-(d-\alpha)} \sum_{\vec{k}, \vec{l}} \frac{s(\vec{k})s(\vec{l})}{|\vec{k} - \vec{l}|^\alpha} + \sum_{\vec{k}} V[s(\vec{k})]. \quad (6)$$

Here the  $s$  are spins which run over a discrete set  $S$ , the indices  $\vec{k}$  run over a  $d$ -dimensional lattice and  $\alpha$  is an exponent between zero and  $d$ . The normalization of the interaction by  $L^{-(d-\alpha)}$  guarantees that the Hamiltonian is in fact *extensive*.

To express the partition function in the form (1), we introduce coarse-grained variables  $m(\vec{x})$  for the magnetization. Using the long-range nature of the interaction, one obtains an expression for the partition function in terms of a functional integral over all  $m(\vec{x})$ . This integral is found to be dominated by a single saddle-point, which corresponds to a function  $m(\vec{x})$  equal to a constant. One can therefore replace the functional integration by an ordinary integration over this constant value and one has cast the partition function in the form (1). For details about this derivation see Ref. [7].

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